

=> d his

-- (FILE 'HOME' ENTERED AT 20:54:36 ON 17 JUN 2001)

FILE 'REGISTRY' ENTERED AT 20:54:45 ON 17 JUN 2001  
L1 STRUCTURE UPLOADED  
L2 1 S L1  
L3 477 S L2 FULL

FILE 'CA' ENTERED AT 20:55:37 ON 17 JUN 2001  
L4 133 S L3  
L5 STRUCTURE UPLOADED  
S L5

FILE 'REGISTRY' ENTERED AT 20:57:28 ON 17 JUN 2001  
L6 1 S L5

FILE 'CA' ENTERED AT 20:57:30 ON 17 JUN 2001  
L7 1 S L6

FILE 'REGISTRY' ENTERED AT 20:57:35 ON 17 JUN 2001  
L8 459 S L5 FULL  
L9 459 S L6 FULL

FILE 'REGISTRY' ENTERED AT 21:01:02 ON 17 JUN 2001  
L10 STRUCTURE UPLOADED  
L11 0 S L10  
L12 1 S L11 FULL

FILE 'CA' ENTERED AT 21:01:38 ON 17 JUN 2001  
L13 2 S L12  
L14 1 S L13 AND BERNARDON, J?/AU  
L15 1 S L13 NOT L14  
L16 0 S L15 AND PD < JULY 1998

FILE 'REGISTRY' ENTERED AT 21:03:39 ON 17 JUN 2001  
L17 STRUCTURE UPLOADED  
L18 0 S L17  
L19 0 S L18 FULL  
L20 STRUCTURE UPLOADED  
L21 0 S L20  
L22 6 S L21 FULL

FILE 'HCAPLUS' ENTERED AT 21:05:16 ON 17 JUN 2001  
L23 16 S L22  
L24 1 S L23 AND BERNARDON, J?/AU  
L25 7 S L23 AND PD < JULY 1998

FILE 'CAOLD' ENTERED AT 21:06:44 ON 17 JUN 2001

=> s 122

L26 0 L22

=>

---Logging off of STN---

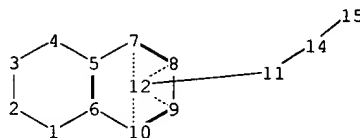
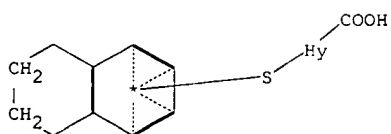
=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.31	851.81
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-5.26

STN INTERNATIONAL LOGOFF AT 21:06:59 ON 17 JUN 2001



chain nodes :

11 14 15

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

11-14 14-15

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds :

11-14 14-15

exact bonds :

1-2 1-6 2-3 3-4 4-5

normalized bonds :

5-6 5-7 6-10 7-8 8-9 9-10

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS

12:CLASS 14:Atom 15:CLASS

Generic attributes :

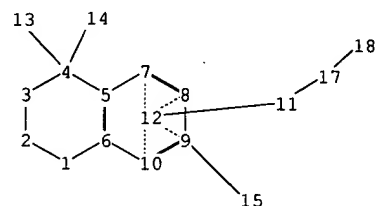
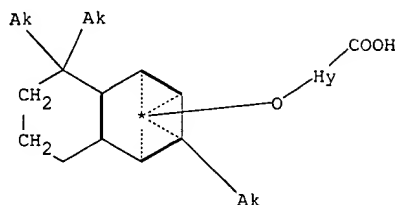
14:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Number of Hetero Atoms : less than 2

Type of Ring System : Monocyclic



chain nodes :

11 13 14 15 17 18

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

4-13 4-14 9-15 11-17 17-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds :

4-13 4-14 9-15 11-17 17-18

exact bonds :

1-2 1-6 2-3 3-4 4-5

normalized bonds :

5-6 5-7 6-10 7-8 8-9 9-10

isolated ring systems :

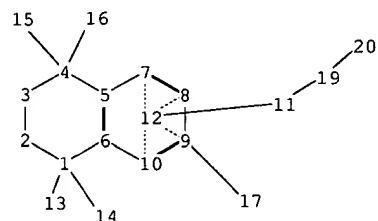
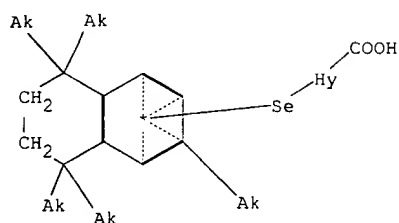
containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS  
12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:Atom 18:CLASS

Generic attributes :

17:  
Saturation : Unsaturated  
Number of Carbon Atoms : less than 7  
Number of Hetero Atoms : less than 2  
Type of Ring System : Monocyclic



chain nodes :

11 13 14 15 16 17 19 20

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

1-14 1-13 4-15 4-16 9-17 11-19 19-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds :

1-14 1-13 4-15 4-16 9-17 11-19 19-20

exact bonds :

1-2 1-6 2-3 3-4 4-5

normalized bonds :

5-6 5-7 6-10 7-8 8-9 9-10

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS

12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:Atom 20:CLASS

Generic attributes :

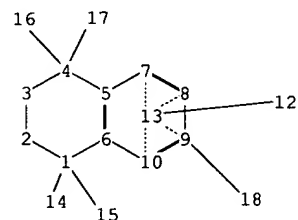
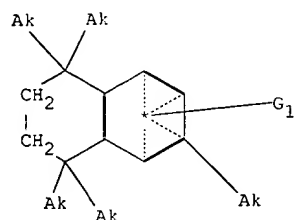
19:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Number of Hetero Atoms : less than 2

Type of Ring System : Monocyclic



chain nodes :

12 14 15 16 17 18

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

1-15 1-14 4-16 4-17 9-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds :

1-15 1-14 4-16 4-17 9-18

exact bonds :

1-2 1-6 2-3 3-4 4-5

normalized bonds :

5-6 5-7 6-10 7-8 8-9 9-10

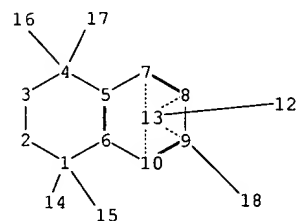
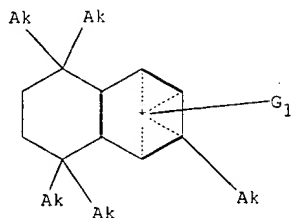
isolated ring systems :

containing 1 :

G1:O,S,Po,Se,Te

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS  
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS



chain nodes :  
 12 14 15 16 17 18  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 10  
 chain bonds :  
 1-15 1-14 4-16 4-17 9-18  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10  
 exact/norm bonds :  
 1-15 1-14 4-16 4-17 9-18  
 exact bonds :  
 1-2 1-6 2-3 3-4 4-5  
 normalized bonds :  
 5-6 5-7 6-10 7-8 8-9 9-10  
 isolated ring systems :  
 containing 1 :

G1:O,S,Po,Se,Te

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS  
 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

Connecting via Winsock to STN

Trying 3106016892...Open

Welcome to STN International! Enter x:x

LOGINID:ssspta1612BXR

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
 NEWS 2 Dec 17 The CA Lexicon available in the CAPLUS and CA files  
 NEWS 3 Feb 06 Engineering Information Encompass files have new names  
 NEWS 4 Feb 16 TOXLINE no longer being updated  
 NEWS 5 Apr 23 Search Derwent WPINDEX by chemical structure  
 NEWS 6 Apr 23 PRE-1967 REFERENCES NOW SEARCHABLE IN CAPLUS AND CA  
 NEWS 7 May 07 DGENE Reload

NEWS EXPRESS May 23 CURRENT WINDOWS VERSION IS V6.0a,  
 CURRENT MACINTOSH VERSION IS V5.0C (ENG) AND V5.0JB (JP),  
 AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2001  
 NEWS HOURS STN Operating Hours Plus Help Desk Availability  
 NEWS INTER General Internet Information  
 NEWS LOGIN Welcome Banner and News Items  
 NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
 NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 20:54:36 ON 17 JUN 2001

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.15	0.15

FILE 'REGISTRY' ENTERED AT 20:54:45 ON 17 JUN 2001

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STRUCTURE FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5

DICTIONARY FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

=>

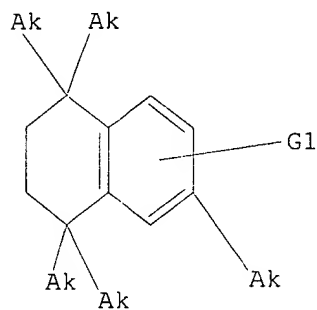
Uploading 09719219.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O, S, Po, Se, Te

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 20:55:17 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 10238 TO ITERATE

9.8% PROCESSED 1000 ITERATIONS 1 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 198709 TO 210811  
PROJECTED ANSWERS: 13 TO 395

L2 1 SEA SSS SAM L1

=> s l2 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 20:55:26 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 205394 TO ITERATE

100.0% PROCESSED 205394 ITERATIONS  
 SEARCH TIME: 00.00.07

477 ANSWERS

L3 477 SEA SSS FUL L1

=> file ca

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	133.56	133.71

FILE 'CA' ENTERED AT 20:55:37 ON 17 JUN 2001  
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FILE COVERS 1947 - 14 Jun 2001 VOL 134 ISS 26  
 FILE LAST UPDATED: 14 Jun 2001 (20010614/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

The CA file now provides online access to patents and literature covered in CA from 1947 to the present. On April 22, 2001, bibliographic information and abstracts were added for over 2.2 million references published in CA from 1947 to 1966.

The CA Lexicon is now available in the Controlled Term (/CT) field. Enter HELP LEXICON for full details.

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=> s l3

L4 133 L3

=>

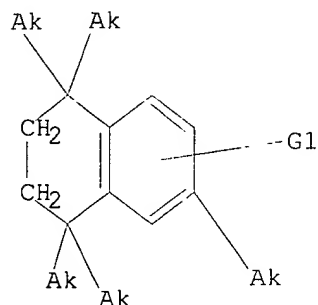
Uploading 9719219a.str

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



G1 O, S, Po, Se, Te

Structure attributes must be viewed using STN Express query preparation.

=> s 15

# **REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 20:57:29 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 10238 TO ITERATE

9.8% PROCESSED 1000 ITERATIONS 1 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 198709 TO 210811  
PROJECTED ANSWERS: 13 TO 395

L6 1 SEA SSS SAM L5

L7 1 L6

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

	ENTRY	SESSION
FULL ESTIMATED COST	0.31	135.26

FILE 'REGISTRY' ENTERED AT 20:57:35 ON 17 JUN 2001  
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STRUCTURE FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5  
 DICTIONARY FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT  
 for details.

=> d his

(FILE 'HOME' ENTERED AT 20:54:36 ON 17 JUN 2001)

FILE 'REGISTRY' ENTERED AT 20:54:45 ON 17 JUN 2001  
 L1 STRUCTURE UPLOADED  
 L2 1 S L1  
 L3 477 S L2 FULL

FILE 'CA' ENTERED AT 20:55:37 ON 17 JUN 2001  
 L4 133 S L3  
 L5 STRUCTURE UPLOADED  
 S L5

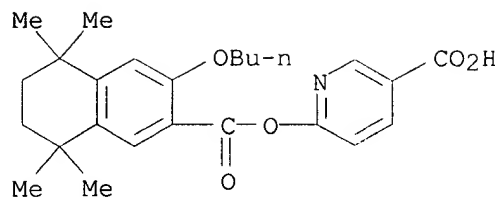
FILE 'REGISTRY' ENTERED AT 20:57:28 ON 17 JUN 2001  
 L6 1 S L5

FILE 'CA' ENTERED AT 20:57:30 ON 17 JUN 2001  
 L7 1 S L6

FILE 'REGISTRY' ENTERED AT 20:57:35 ON 17 JUN 2001

=> d 16

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2001 ACS  
 RN 191157-30-9 REGISTRY  
 CN 3-Pyridinecarboxylic acid, 6-[[ (3-butoxy-5,6,7,8-tetrahydro-5,5,8,8-  
 tetramethyl-2-naphthalenyl)carbonyl]oxy]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C25 H31 N O5  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> s 15 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 20:58:03 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 205394 TO ITERATE

100.0% PROCESSED 205394 ITERATIONS 459 ANSWERS  
SEARCH TIME: 00.00.07

L8 459 SEA SSS FUL L5

=> s 16 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 20:58:30 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 205394 TO ITERATE

100.0% PROCESSED 205394 ITERATIONS 459 ANSWERS  
SEARCH TIME: 00.00.06

L9 459 SEA SSS FUL L5

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	269.86	405.12

FILE 'REGISTRY' ENTERED AT 21:01:02 ON 17 JUN 2001  
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TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

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Structure search limits have been increased. See HELP SLIMIT for details.

=>

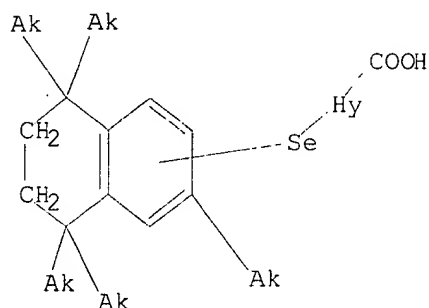
Uploading 9719219c.str

L10 STRUCTURE UPLOADED

=> d l10

L10 HAS NO ANSWERS

L10 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l10

SAMPLE SEARCH INITIATED 21:01:23 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2 TO 124  
PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=> s l11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 21:01:29 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 104 TO ITERATE

100.0% PROCESSED 104 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

L12 1 SEA SSS FUL L10

=> file ca

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	133.56	538.68

FILE 'CA' ENTERED AT 21:01:38 ON 17 JUN 2001  
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FILE COVERS 1947 - 14 Jun 2001 VOL 134 ISS 26  
 FILE LAST UPDATED: 14 Jun 2001 (20010614/ED)

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=> s l12

L13 2 L12

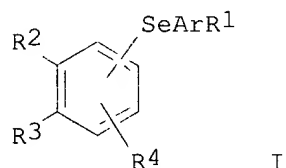
=> s l13 and bernardon, j?/au

58 BERNARDON, J?/AU  
 L14 1 L13 AND BERNARDON, J?/AU

=> d l14, ibib abs hitstr, 1

L14 ANSWER 1 OF 1 CA COPYRIGHT 2001 ACS  
 ACCESSION NUMBER: 132:35910 CA  
 TITLE: Preparation of diaryl selenide compounds and their use  
 in human or veterinary medicine and in cosmetics  
 INVENTOR(S): **Bernardon, Jean-Michel; Diaz, Philippe**  
 PATENT ASSIGNEE(S): Galderma Research & Development, S.N.C., Fr.  
 SOURCE: PCT Int. Appl., 81 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9965872	A1	19991223	WO 1999-FR1389	19990611
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
FR 2779720	A1	19991217	FR 1998-7439	19980612
AU 9940491	A1	20000105	AU 1999-40491	19990611
EP 1086080	A1	20010328	EP 1999-923723	19990611
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
NO 2000006337	A	20010212	NO 2000-6337	20001212
PRIORITY APPLN. INFO.:			FR 1998-7439	A 19980612
			WO 1999-FR1389	W 19990611
OTHER SOURCE(S):	MARPAT 132:35910			
GI				

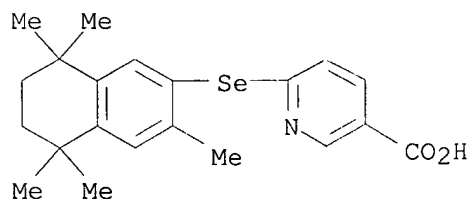


AB The invention concerns novel diaryl selenide compds. corresponding to I and their geometric and optical isomers and salts and the use thereof in pharmaceutical compns. in human or veterinary medicine (in the treatment of dermatol., rheumatic, cardiovascular and ophthalmol. pathologies in particular), or in cosmetic compns. In I, R1 = Me, CH2OR5 (R5 = H, lower alkyl, C(O)R10 (R10 = lower alkyl)), C(O)R6 (R6 = H, lower alkyl, OR12 (R12 = H, lower alkyl, aryl, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl), NR'R'' (R'/R'' = H, lower alkyl, aryl

possibly substituted, amino acid fragment; R' and R'' together with N form a heterocycle)); Ar = R7-substituted benzene or pyridine diradical (R7 = H, halogen, lower alkyl, nitro, OR13 (R13 = H, lower alkyl), polyether radical, NR14R15 (R14/R15 = H, lower alkyl)), diradicals of furan, thiophene or thiazole; R2/R3 = H, tBu, 1-methylcyclohexyl, 1-adamantyl, OR8 (R8 = H, lower alkyl, aryl possibly substituted, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl, lower alkyl), polyether radical, where at least one of R2 or R3 = tBu, 1-methylcyclohexyl, 1-adamantyl; R2 and R3 may together with an adjacent arom. ring form a satd. 5- or 6-membered ring possibly substituted by Me groups and/or possibly interrupted by O or S; R4 = H, halogen, lower alkyl, OR9 (R9 = H, lower alkyl, aryl possibly substituted, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl, lower alkyl, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R16 (R16 = H, lower alkyl; n = 1-12), (CH<sub>2</sub>)<sub>n</sub>X (X = halogen)), polyether radical, C(O)R10. Although the method of prepn. is not claimed, 70 example prepn. are included. In a typical prepn., a haloarene (e.g. 2-bromo-5,6,7,8-tetrahydro-3,5,5,8,8-pentamethylnaphthalene) is successively reacted with tBuLi in THF, Se, and NaOH in EtOH to give a diselenide, which is cleaved with NaBH<sub>4</sub> in EtOH to give the Na salt of an areneselenol, which is undergoes metathesis with IR1 or BrR1 (e.g. Et 4-iodobenzoate) in the presence of NiBr<sub>2</sub>py<sub>2</sub> in EtOH to give I (e.g. Et 4-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-ylselenenyl)benzoate).

IT 52352-76-4, 6-(3,5,5,8,8-Pentamethyl-5,6,7,8-tetrahydronaphthalen-2-ylselenenyl)nicotinic acid  
 RL: RCT (Reactant)  
 (reactant; prepn. of diaryl selenide compds. and use in human or veterinary medicine and in cosmetics)

RN 252352-76-4 CA  
 CN 3-Pyridinecarboxylic acid,  
 6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)seleno]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13  
 REFERENCE(S): (1) Allergan Inc; WO 9716422 A 1997 CA  
 (2) Bernardon, J; WO 9822423 A 1998 CA  
 (3) Boehm, M; Journal of Medicinal Chemistry 1995, V38, P3146 CA  
 (4) Cird; WO 9220643 A 1992 CA  
 (5) Cird, G; EP 0661258 A 1995 CA  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 20:54:36 ON 17 JUN 2001)

FILE 'REGISTRY' ENTERED AT 20:54:45 ON 17 JUN 2001

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 477 S L2 FULL

FILE 'CA' ENTERED AT 20:55:37 ON 17 JUN 2001

L4 133 S L3

L5 STRUCTURE UPLOADED

S L5

FILE 'REGISTRY' ENTERED AT 20:57:28 ON 17 JUN 2001

L6 1 S L5

FILE 'CA' ENTERED AT 20:57:30 ON 17 JUN 2001

L7 1 S L6

FILE 'REGISTRY' ENTERED AT 20:57:35 ON 17 JUN 2001

L8 459 S L5 FULL

L9 459 S L6 FULL

FILE 'REGISTRY' ENTERED AT 21:01:02 ON 17 JUN 2001

L10 STRUCTURE UPLOADED

L11 0 S L10

L12 1 S L11 FULL

FILE 'CA' ENTERED AT 21:01:38 ON 17 JUN 2001

L13 2 S L12

L14 1 S L13 AND BERNARDON, J?/AU

=> s 113 not 114

L15 1 L13 NOT L14

=> s 115 and pd < july 1998

17097245 PD < JULY 1998  
(PD<19980700)

L16 0 L15 AND PD < JULY 1998

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.88	546.56
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.56	-0.56

FILE 'REGISTRY' ENTERED AT 21:03:39 ON 17 JUN 2001

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STRUCTURE FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5  
DICTIONARY FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT  
for details.

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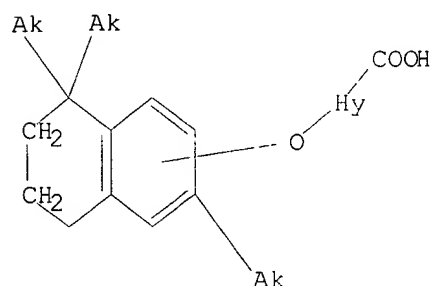
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L17 STRUCTURE UPLOADED

=> d l17

L17 HAS NO ANSWERS

L17 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l17

SAMPLE SEARCH INITIATED 21:03:59 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 1872 TO ITERATE

53.4% PROCESSED 1000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 34846 TO 40034  
PROJECTED ANSWERS: 0 TO 0

L18 0 SEA SSS SAM L17

=> s l18 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 21:04:04 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 37574 TO ITERATE

100.0% PROCESSED 37574 ITERATIONS  
SEARCH TIME: 00.00.02

0 ANSWERS

L19 0 SEA SSS FUL L17

=>

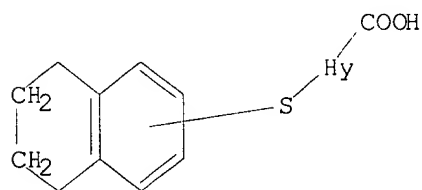
Uploading 9719219e.str

L20 STRUCTURE UPLOADED

=> d 120

L20 HAS NO ANSWERS

L20 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 120

SAMPLE SEARCH INITIATED 21:05:03 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 1872 TO ITERATE

53.4% PROCESSED 1000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 34846 TO 40034  
PROJECTED ANSWERS: 0 TO 0

L21 0 SEA SSS SAM L20

=> s 121 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 21:05:08 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 37574 TO ITERATE

100.0% PROCESSED 37574 ITERATIONS  
SEARCH TIME: 00.00.03

6 ANSWERS

L22 6 SEA SSS FUL L20

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	267.43	813.99
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.56

FILE 'HCAPLUS' ENTERED AT 21:05:16 ON 17 JUN 2001  
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FILE COVERS 1947 - 17 Jun 2001 VOL 134 ISS 26  
FILE LAST UPDATED: 15 Jun 2001 (20010615/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

HCAplus now provides online access to patents and literature covered in CA from 1947 to the present. On April 22, 2001, bibliographic information and abstracts were added for over 2.2 million references published in CA from 1947 to 1966.

=> s l22

L23 16 L22

=> s l23 and bernardon, j?/au

61 BERNARDON, J?/AU  
L24 1 L23 AND BERNARDON, J?/AU

=> d l24, ibib abs hitstr, 1

L24 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1995:995753 HCAPLUS

DOCUMENT NUMBER: 124:145647

TITLE: Preparation of (tetrahydronaphthyloxy)benzoates and analogs as cell proliferation inhibitors

INVENTOR(S): Bernardon, Jean-Michel

PATENT ASSIGNEE(S): Centre International de Recherches Dermatologiques Galderma (C.I.R.D. Galderma), Fr.

SOURCE: Eur. Pat. Appl., 22 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

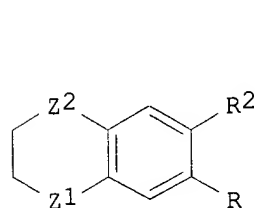
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

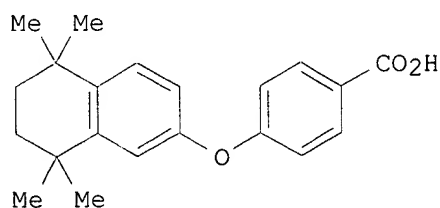
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 679630	A1	19951102	EP 1995-400701	19950329
EP 679630	B1	19980506		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT,				
SE				
FR 2719043	A1	19951027	FR 1994-5019	19940426
FR 2719043	B1	19960531		
AT 165807	E	19980515	AT 1995-400701	19950329
ES 2119326	T3	19981001	ES 1995-400701	19950329
ZA 9502974	A	19951219	ZA 1995-2974	19950411
AU 9516512	A1	19951116	AU 1995-16512	19950418
AU 668495	B2	19960502		
NO 9501545	A	19951027	NO 1995-1545	19950424
CA 2147807	AA	19951027	CA 1995-2147807	19950425
FI 9501967	A	19951027	FI 1995-1967	19950425
JP 08169857	A2	19960702	JP 1995-101512	19950425
HU 74014	A2	19961028	HU 1995-1167	19950425
BR 9501612	A	19970916	BR 1995-1612	19950425
RU 2141471	C1	19991120	RU 1995-106680	19950425
PL 179902	B1	20001130	PL 1995-308343	19950425
US 5766610	A	19980616	US 1995-429096	19950426
US 6015569	A	20000118	US 1997-971983	19971117
US 6162815	A	20001219	US 1998-150727	19980910
US 6156788	A	20001205	US 1999-369875	19990809
PRIORITY APPLN. INFO.:			FR 1994-5019	A 19940426
			US 1995-429096	A1 19950426
			US 1997-971983	A2 19971117

OTHER SOURCE(S): MARPAT 124:145647

GI



I



II

AB Title compds. [I; R = ZR1; R1 = (un)substituted Ph, -heterocyclyl; R2 = H,

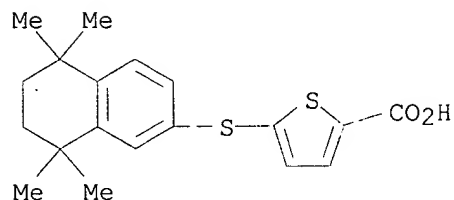
halo, alkyl, etc.; Z = O, SOO-2, (alkyl)imino; Z1,Z2 = O, SOO-2, (di)(alkyl)methylene] were prepd. as cell proliferation inhibitors (no data). Thus, 5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthol was etherified by 4-IC6H4CO2Me and the product sapond. to give title compd. II.

IT 173156-90-6P 173156-98-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of (tetrahydronaphthyl)benzoates and analogs as cell proliferation inhibitors)

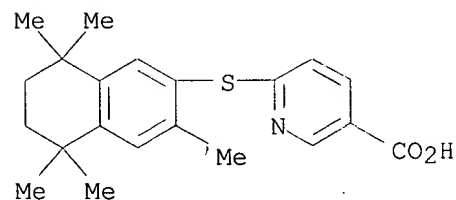
RN 173156-90-6 HCAPLUS

CN 2-Thiophenecarboxylic acid, 5-[(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)thio]- (9CI) (CA INDEX NAME)



RN 173156-98-4 HCAPLUS

CN 3-Pyridinecarboxylic acid, 6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)thio]- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 20:54:36 ON 17 JUN 2001)

FILE 'REGISTRY' ENTERED AT 20:54:45 ON 17 JUN 2001

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 477 S L2 FULL

FILE 'CA' ENTERED AT 20:55:37 ON 17 JUN 2001

L4 133 S L3  
 L5 STRUCTURE UPLOADED  
 S L5

FILE 'REGISTRY' ENTERED AT 20:57:28 ON 17 JUN 2001  
 L6 1 S L5

FILE 'CA' ENTERED AT 20:57:30 ON 17 JUN 2001  
 L7 1 S L6

FILE 'REGISTRY' ENTERED AT 20:57:35 ON 17 JUN 2001  
 L8 459 S L5 FULL  
 L9 459 S L6 FULL

FILE 'REGISTRY' ENTERED AT 21:01:02 ON 17 JUN 2001  
 L10 STRUCTURE UPLOADED  
 L11 0 S L10  
 L12 1 S L11 FULL

FILE 'CA' ENTERED AT 21:01:38 ON 17 JUN 2001  
 L13 2 S L12  
 L14 1 S L13 AND BERNARDON, J?/AU  
 L15 1 S L13 NOT L14  
 L16 0 S L15 AND PD < JULY 1998

FILE 'REGISTRY' ENTERED AT 21:03:39 ON 17 JUN 2001  
 L17 STRUCTURE UPLOADED  
 L18 0 S L17  
 L19 0 S L18 FULL  
 L20 STRUCTURE UPLOADED  
 L21 0 S L20  
 L22 6 S L21 FULL

FILE 'HCAPLUS' ENTERED AT 21:05:16 ON 17 JUN 2001  
 L23 16 S L22  
 L24 1 S L23 AND BERNARDON, J?/AU

=> s l23 and pd < july 1998

17383507 PD < JULY 1998  
 (PD<19980700)  
 L25 7 L23 AND PD < JULY 1998

=> d l25, ibib abs fhitr, 1-7

L25 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2001 ACS  
 ACCESSION NUMBER: 1998:728106 HCAPLUS  
 DOCUMENT NUMBER: 130:104932  
 TITLE: ET-1 expression and growth inhibition of prostate  
 cancer cells: a retinoid target with novel  
 specificity  
 AUTHOR(S): Hsu, Ju-Yu; Pfahl, Magnus  
 CORPORATE SOURCE: Sidney Kimmel Cancer Center, San Diego, CA, 92121,  
 USA  
 SOURCE: Cancer Res. (1998), 58(21), 4817-4822

CODEN: CNREA8; ISSN: 0008-5472  
 PUBLISHER: AACR Subscription Office  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Endothelin-1 (ET-1) is not only a potent vasoconstrictor but also serves as an important growth stimulator in various cancers, including breast, cervical, pancreatic, and prostate cancer. This suggests that blockage of

ET-1 prodn. may suppress tumor growth and possibly metastasis. The authors obsd. that certain synthetic retinoids and all-trans-retinoic acid

can repress LNCaP prostate cancer cell growth in vitro. In addn., these retinoid compds. counteracted exogenous ET-1-induced growth stimulation. Retinoid-dependent growth retardation of LNCaP cells coincided with suppression of ET-1 gene expression to a level undetectable by reverse transcription-PCR. Contrarily, the androgen-insensitive DU145 cells were refractory to retinoid treatment. To investigate the underlying mechanisms of the cell-specific response to retinoids, the authors transfected ET-1 promoter constructs contg. wild-type or mutated AP-1 or GATA-2 site into prostate cancer cells. Distinct regulations of ET-1 promoter activity were found; in LNCaP cells, both binding sites are essential for optimal promoter activation, whereas in DU145 cells, addnl. promoter sequences and/or transcriptional factors seem to be involved. Furthermore, several anti-AP-1 selective retinoids failed to repress ET-1 promoter activity and to exhibit a cell growth-inhibitory effect on LNCaP cells, suggesting that different retinoid structural configurations are required for the inhibition of an AP-1 complex vs. an AP-1/GATA-2

complex.

IT 173156-98-4, CD 2809

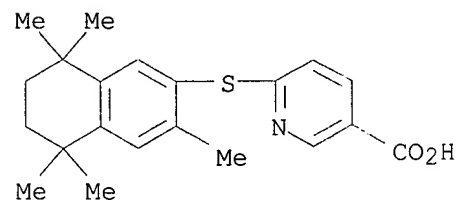
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(endothelin 1 expression and growth inhibition of prostate cancer cells

response to retinoids in relation to AP-1 and GATA-2 sites in endothelin 1 promoter)

RN 173156-98-4 HCAPLUS

CN 3-Pyridinecarboxylic acid,  
 6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)thio]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25

REFERENCE(S): (3) Baley, P; J Clin Invest 1990, V85, P1320 HCAPLUS  
 (4) Benatti, L; J Clin Invest 1993, V91, P1149

HCAPLUS

(5) Blutt, S; Endocrinology 1997, V138, P1491 HCAPLUS  
 (6) Dawson, M; Cancer Res 1995, V55, P4446 HCAPLUS

(7) Dawson, M; J Med Chem 1995, V38, P3368 HCAPLUS  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:206286 HCAPLUS

DOCUMENT NUMBER: 128:317589

TITLE: Inhibition of the 1,25-dihydroxyvitamin D3-induced increase in vitamin D receptor (VDR) levels and binding of VDR-retinoid X receptor (RXR) to a direct repeat (DR)-3 type response element by an

RXR-specific

ligand in human keratinocyte cultures  
AUTHOR(S): Jensen, Tina J.; Henriksen, Linda O.; Solvsten, Henrik; Kragballe, Knud  
CORPORATE SOURCE: DEPARTMENT OF DERMATOLOGY, MARSELISHORG HOSPITAL, AARHUS C, DK-8000, Den.  
SOURCE: Biochem. Pharmacol. (1998), 55(6), 767-773  
CODEN: BCPA6; ISSN: 0006-2952

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The biol. active form of vitamin D, 1,25-dihydroxyvitamin D3 (1,25(OH)2D3), mediates most of its actions through the intracellular vitamin D receptor (VDR). VDR binds to vitamin D responsive elements (VDREs) in the promoter region of responsive genes and regulates transcription. Usually the VDREs consist of a direct repeat of two hexanucleotides spaced by three nucleotides (DR-3), to which VDR preferentially binds as a heterodimer with the retinoid X receptor (RXR). In the present study, we examd. the effect of 1,25(OH)2D3 and a specific ligand for RXR, CD2809, on VDR and RXR levels in cultured human keratinocytes and on the binding of RXR-VDR to a DR-3 type response element. Incubation with 1,25(OH)2D3 increased VDR levels as detd. by Western blotting, increased VDR-RXR binding to a DR-3 type response element as detd. by the electromobility shift assay (EMSA), and induced the 25-OH-D3 24-hydroxylase (24-hydroxylase) gene, contg. a DR-3 type response element. CD2809 caused a slight decrease in RXR.alpha. levels, but had no effect on VDR levels. Addn. of both CD2809 and 1,25(OH)2D3 decreased VDR levels as well as the VDR-RXR binding levels to the DR-3 type response element, compared to 1,25(OH)2D3 alone. In conclusion, an RXR-specific ligand interferes with the 1,25(OH)2D3-induced stimulation

of VDR levels and VDR-RXR binding to DNA in keratinocyte cultures. It is therefore possible that RXR-specific ligands may counteract certain biol. actions of vitamin D3-.

IT 173156-98-4, CD2809

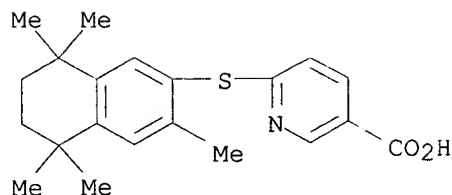
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(dihydroxyvitamin D3 effect on VDR and RXR.alpha. levels and the binding of VDR-RXR to a direct repeat (DR)-3 type response element in relation to costimulatory effects of the RXR-specific ligand CD2809)

RN 173156-98-4 HCAPLUS

CN 3-Pyridinecarboxylic acid,

6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)thio]- (9CI) (CA INDEX NAME)



L25 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1998:175698 HCAPLUS

DOCUMENT NUMBER: 128:213396

TITLE: Use of retinoids for the preparation of a medicament for treating disorders related to VEGF overexpression  
 INVENTOR(S): Vega, Barbara; Michel, Serge; Ladoux, Annie; Frelin, Christian

PATENT ASSIGNEE(S): Centre International de Recherches Dermatologiques Galderma, (Cird Galderma), Fr.

SOURCE: Eur. Pat. Appl., 9 pp.

CODEN: EPXXDW

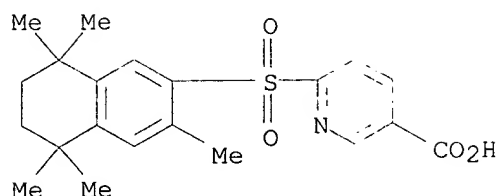
DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 826368	A1	19980304	EP 1997-401998	19970827 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
FR 2752734	A1	19980306	FR 1996-10685	19960902 <--
FR 2752734	B1	19981106		
CA 2213690	AA	19980302	CA 1997-2213690	19970829 <--
AU 9736090	A1	19980305	AU 1997-36090	19970829 <--
AU 712750	B2	19991118		
BR 9702808	A	19990105	BR 1997-2808	19970829
JP 10087481	A2	19980407	JP 1997-236308	19970901 <--
JP 3107775	B2	20001113		
US 6001885	A	19991214	US 1997-921511	19970902
PRIORITY APPLN. INFO.: FR 1996-10685 A 19960902				
AB Retinoids, particularly anti-AP1 are used for the prepn. of a medicament for treating disorders related to VEGF (vascular endothelial growth factor) overexpression, e.g. psoriasis and Kaposi syndrome. Thus, 6-[3-(1-adamantyl)-4-methoxyphenyl]2-naphthoic acid at 10 <sup>-8</sup> M concn. inhibited the expression of VEGF in cultured keratinocytes by 58% as compared with glyceraldehyde phosphate dehydrogenase.				
IT 204332-26-3				
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (use of retinoids for prepn. of medicament for treating disorders related to VEGF overexpression)				
RN 204332-26-3 HCAPLUS				
CN 3-Pyridinecarboxylic acid, 6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)sulfonyl]- (9CI) (CA INDEX NAME)				



L25 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:549073 HCAPLUS

DOCUMENT NUMBER: 127:243238

TITLE: Effects of vitamin D3 on keratinocyte proliferation and differentiation in vitro. Modulation by ligands for retinoic acid and retinoid X receptors

AUTHOR(S): Sorensen, S.; Solvsten, H.; Politi, Y.; Kragballe, Knut

CORPORATE SOURCE: Marselisborg Hospital, University Aarhus, Aarhus, DK-8000, Den.

SOURCE: Skin Pharmacol. (1997), 10(3), 144-152

CODEN: SKPHEU; ISSN: 1011-0283

PUBLISHER: Karger

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The antiproliferative and prodifferentiating effects of 1,25-dihydroxyvitamin D3 (1,25(OH)2D3) on normal human keratinocyte cultures were investigated after incubation for 4 days with the ligands all-trans-retinoic acid (all-trans RA), CD2809, 9-cis-retinoic acid (9-cis-RA), and triiodothyronine (T3). Proliferation was measured by the dimethylthiazolyl-diphenyl-tetrazolium-bromide assay and differentiation was detd. in the same culture with a cell ELISA for transglutaminase type I. All-trans RA, 9-cis-RA, and CD2809 had a slight stimulatory effect on proliferation. In combination with 1,25(OH)2D3, all retinoids partially counteracted the antiproliferative effect of 1,25(OH)2D3. The differentiation was inhibited dose-dependently by all-trans RA, 9-cis-RA, and CD2809. In combination with 1,25(OH)2D3, all retinoids reversed the prodifferentiating effects of 1,25(OH)2D3 resulting in a net inhibition

of differentiation. T3 alone or in combination with 1,25(OH)2D3 had no effect on proliferation or differentiation. Ligand-dependent heterodimer formation between the vitamin D receptor and retinoid receptors may not

be important for the combined effects of 1,25(OH)2D3 and retinoids on keratinocyte proliferation and differentiation in vitro.

IT 173156-98-4, CD 2809

RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(effects of vitamin D3 on keratinocyte proliferation and differentiation, modulation by ligands for retinoic acid and retinoid

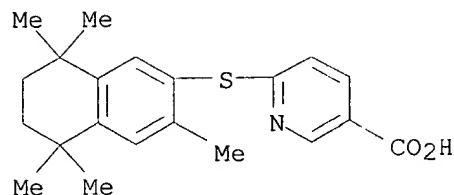
X receptors)

RN 173156-98-4 HCAPLUS

CN 3-Pyridinecarboxylic acid,

6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-

naphthalenyl)thio]- (9CI) (CA INDEX NAME)



L25 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:403183 HCAPLUS

DOCUMENT NUMBER: 127:17489

TITLE: Preparation of tetrahydronaphthylthiobenzoates and analogs as retinoid X receptor agonists

INVENTOR(S): Beard, Richard L.; Colon, Diana F.; Chandraratna, Roshantha A.

PATENT ASSIGNEE(S): Allergan, USA

SOURCE: PCT Int. Appl., 49 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

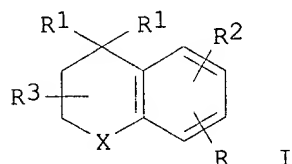
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

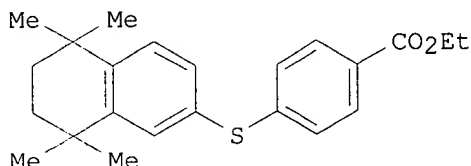
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9716422	A1	19970509	WO 1996-US17295	19961029 <--
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RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
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US 5672710	A	19970930	US 1995-552965	19951101 <--
PRIORITY APPLN. INFO.: US 1995-552965 19951101				
WO 1996-US17295 19961029				

OTHER SOURCE(S): MARPAT 127:17489  
GI



I



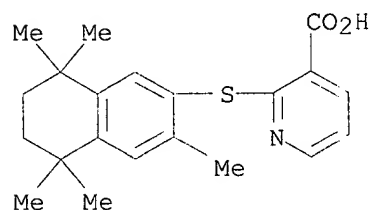
II

AB Title compds. [I; R = SOO-2ZAB; A = bond, alk(en)ylene, alkynylene; B = H,

CH<sub>2</sub>OH, alkoxy carbonyl, etc.; R<sub>1</sub> = H or alkyl; R<sub>2</sub> = 1-3 substituents selected from H, halo, alkyl, alkoxy, etc.; R<sub>3</sub> = 1-4 substituents selected from H, F, alkyl; X = O, S, (alkyl)imino, CH<sub>2</sub>, etc.; Z = (un)substituted phenylene, -heteroarylene] were prepd. Thus, 5,6,7,8-tetrahydro-5,5,8,8-tetramethylnaphthalene-2-thiol was thioetherified by 4-IC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Et to give title compd. II. Data for biol. activity of I were given.

IT **190596-59-9P**  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of tetrahydronaphthylthiobenzoates and analogs as retinoid X receptor agonists)

RN 190596-59-9 HCAPLUS  
 CN 3-Pyridinecarboxylic acid,  
 2-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)thio]- (9CI) (CA INDEX NAME)



103

L25 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2001 ACS  
 ACCESSION NUMBER: 1996:483612 HCAPLUS  
 DOCUMENT NUMBER: 125:131667  
 TITLE: Synthesis and Structure-Activity Relationships of Retinoid X Receptor Selective Diaryl Sulfide Analogs of Retinoic Acid  
 AUTHOR(S): Beard, Richard L.; Colon, Diana F.; Song, Tae K.; Davies, Peter J. A.; Kochhar, Devendra M.; Chandraratna, Roshantha A. S.  
 CORPORATE SOURCE: Department of Chemistry, Allergan Incorporated, Irvine, CA, 92715-1599, USA  
 SOURCE: J. Med. Chem. (1996), 39(18), 3556-3563  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Retinoids exert their biol. effects by binding to and activating nuclear receptors that interact with responsive elements on DNA to promote gene transcription. There are two families of retinoid receptors, the retinoic acid receptor (RAR) family and the retinoid X receptor (RXR) family, which are each further divided into three subclasses: RAR.alpha., .beta., .gamma. and RXR.alpha., .beta., .gamma.. Herein we describe the synthesis and structure-activity relationships SAR of a new series of diaryl sulfide retinoid analogs that specifically bind and transactivate the RXRs. Furthermore, the sulfoxide and sulfone derivs. of these analogs are partial agonists which activate the RXRs only at high concns. Thus, these

compds. possess a potential site of metabolic deactivation and may have less prolonged systemic effects than other compds. with arotinoid-like structures. We show also that these compds. have activity in nontransfected cells as demonstrated by their ability to induce TGase activity in HL-60 cells. Finally, we corroborate our earlier report that RXR-specific agonists may possess reduced teratogenic toxicity compared to

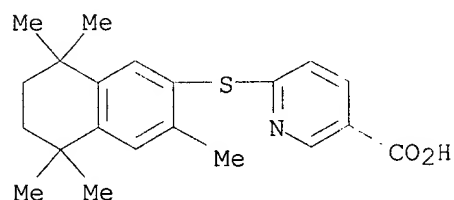
RAR-specific agonists since these compds. are much less potent inhibitors of chondrogenesis than RAR-specific agonists such as TTNPB.

IT 173156-98-4P

RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(synthesis and structure-activity relationships of retinoid x receptor selective diaryl sulfide analogs of retinoic acid)

RN 173156-98-4 HCAPLUS

CN 3-Pyridinecarboxylic acid,  
6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)thio]- (9CI) (CA INDEX NAME)



103

L25 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1995:995753 HCAPLUS

DOCUMENT NUMBER: 124:145647

TITLE: Preparation of (tetrahydronaphthyloxy)benzoates and analogs as cell proliferation inhibitors

INVENTOR(S): Bernardon, Jean-Michel

PATENT ASSIGNEE(S): Centre International de Recherches Dermatologiques Galderma (C.I.R.D. Galderma), Fr.

SOURCE: Eur. Pat. Appl., 22 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

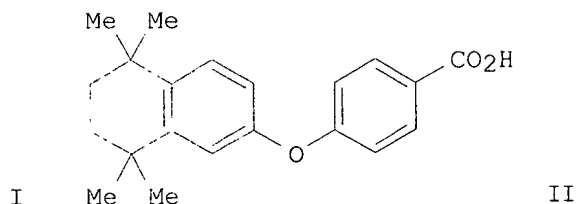
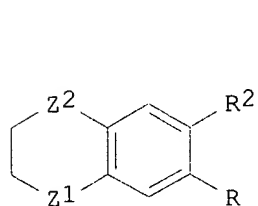
LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 679630	A1	19951102	EP 1995-400701	19950329 <--
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FR 2719043	B1	19960531		
AT 165807	E	19980515	AT 1995-400701	19950329 <--
ES 2119326	T3	19981001	ES 1995-400701	19950329

ZA 9502974	A	19951219	ZA 1995-2974	19950411 <--
AU 9516512	A1	19951116	AU 1995-16512	19950418 <--
AU 668495	B2	19960502		
NO 9501545	A	19951027	NO 1995-1545	19950424 <--
CA 2147807	AA	19951027	CA 1995-2147807	19950425 <--
FI 9501967	A	19951027	FI 1995-1967	19950425 <--
JP 08169857	A2	19960702	JP 1995-101512	19950425 <--
HU 74014	A2	19961028	HU 1995-1167	19950425 <--
BR 9501612	A	19970916	BR 1995-1612	19950425 <--
RU 2141471	C1	19991120	RU 1995-106680	19950425
PL 179902	B1	20001130	PL 1995-308343	19950425
US 5766610	A	19980616	US 1995-429096	19950426 <--
US 6015569	A	20000118	US 1997-971983	19971117
US 6162815	A	20001219	US 1998-150727	19980910
US 6156788	A	20001205	US 1999-369875	19990809
PRIORITY APPLN. INFO.:			FR 1994-5019	A 19940426
			US 1995-429096	A1 19950426
			US 1997-971983	A2 19971117
OTHER SOURCE(S):			MARPAT 124:145647	
GI				



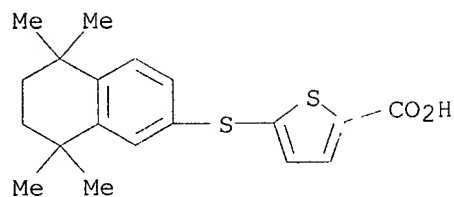
AB Title compds. [I; R = ZR1; R1 = (un)substituted Ph, -heterocyclyl; R2 = H, halo, alkyl, etc.; Z = O, SOO-2, (alkyl)imino; Z1,Z2 = O, SOO-2, (di)(alkyl)methylene] were prepd. as cell proliferation inhibitors (no data). Thus, 5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthol was etherified by 4-IC6H4CO2Me and the product sapond. to give title compd. II.

IT **173156-90-6P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of (tetrahydronaphthyloxy)benzoates and analogs as cell proliferation inhibitors)

RN 173156-90-6 HCAPLUS

CN 2-Thiophenecarboxylic acid, 5-[(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)thio]- (9CI) (CA INDEX NAME)



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L15                  1 S L13 NOT L14

L16                  0 S L15 AND PD < JULY 1998

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L22                  6 S L21 FULL

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L25                  7 S L23 AND PD < JULY 1998

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